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# BMO Martingales and Positive Solutions of Heat Equations

Ying Hu\* and Zhongmin Qian†

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## Abstract

In this paper, we develop a new approach to establish gradient estimates for positive solutions to the heat equation of elliptic or subelliptic operators on Euclidean spaces or on Riemannian manifolds. More precisely, we give some estimates of the gradient of logarithm of a positive solution via the uniform bound of the logarithm of the solution. Moreover, we give a generalized version of Li-Yau's estimate. Our proof is based on the link between PDE and quadratic BSDE. Our method might be useful to study some (nonlinear) PDEs.

## 1 Introduction

In this article, we study positive solutions  $u$  of a linear parabolic equation

$$\left(L - \frac{\partial}{\partial t}\right)u = 0 \quad \text{in } (0, \infty) \times M, \quad (1.1)$$

where  $M$  is either the Euclidean space  $\mathbb{R}^n$  and  $L$  is an elliptic or sub-elliptic operator of second-order  $L = \frac{1}{2} \sum_{\alpha=1}^m A_\alpha^2 + A_0$ ,  $\{A_0, \dots, A_m\}$  is a family of vector fields on  $\mathbb{R}^n$ , or  $M$  is a complete manifold of dimension  $n$  with Riemannian metric  $(g_{ij})$ , and  $2L$  is the Laplace-Beltrami operator

$$\Delta = \frac{1}{\sqrt{g}} \sum_{i,j=1}^n \frac{\partial}{\partial x^i} \sqrt{g} g^{ij} \frac{\partial}{\partial x^j},$$

where  $g$  denotes the determinate of  $(g_{ij})$  and  $(g^{ij})$  is the inverse of the matrix  $(g_{ij})$ .

The well-posedness and the regularity theory for (1.1) are parts of the classical theory in partial differential equations, see [19], [14] and [22] for details. On the other hand, it remains an interesting question to devise precise estimates of a solution  $u$  in terms of the (geometric) structures of (1.1). There is already a large number of papers devoted to this question. Among many interesting results, let us cite two of them which are most relevant to the present paper. The first result is a classical result under the name of semigroup domination, first discovered by Donnelly and Li [8], which says that if the Ricci curvature is bounded from below by  $C$ , then

$$|\nabla P_t u_0| \leq e^{-Ct} P_t |\nabla u_0|, \quad \text{for } u_0 \in C_b^1(M), \quad (1.2)$$

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\*IRMAR, Université Rennes 1, 35042 Rennes Cedex, France. Email: ying.hu@univ-rennes1.fr. This author is partially supported by the Marie Curie ITN Grant, "Controlled Systems", GA no.213841/2008.

†Mathematical Institute, University of Oxford, Oxford OX2 6GG, England. Email: qianz@maths.ox.ac.uk.

where  $(P_t)_{t \geq 0}$  is the heat semigroup on  $M$ , so that the left-hand side is the norm of the gradient of  $u(t, \cdot) = P_t u_0$  a solution to the heat equation

$$\left(\frac{1}{2}\Delta - \frac{\partial}{\partial t}\right)u = 0 \quad \text{in } (0, \infty) \times M \quad (1.3)$$

with initial data  $u(0, \cdot) = u_0$ , while the right-hand side  $P_t |\nabla u_0|$  is a solution of (1.3) with initial data  $|\nabla u_0|$ . The second result is Li-Yau's estimate first established in [20]. If the Ricci curvature is non-negative, and if  $u$  is a positive solution of (1.3) then

$$|\nabla \log u|^2 - 2 \frac{\partial}{\partial t} \log u \leq \frac{n}{t} \quad \text{for } t > 0. \quad (1.4)$$

In fact, in the same paper [20], Li and Yau also obtained a gradient estimate for positive solutions in terms of the dimension and a lower bound (which may be negative) of the Ricci curvature, though less precise. Their estimates in negative case have been improved over the years, see for example [27], [28], [2] and [1].

In this paper we prove several gradient estimates for the positive solutions of (1.1). Let us first mention some simple ones for illustration.

**Theorem 1.1** *Let  $M$  be a complete manifold with non-negative Ricci curvature. Suppose  $u$  is a positive solution of (1.3) with initial data  $u_0 > 0$ , then*

$$|\nabla \log u(t, \cdot)|^2 \leq \frac{4}{t} \|\log u_0\|_\infty, \quad \text{for } t > 0, \quad (1.5)$$

where  $\|\cdot\|_\infty$  denotes the  $L^\infty$  norm on  $M$ .

**Remark 1.2** *As pointed out by the referee, (1.5) can be derived from the reverse logarithmic Sobolev inequality due to Bakry and Ledoux [1]. In fact, from the reverse logarithmic Sobolev inequality,*

$$t P_t(u_0)(x) |\log P_t(u_0)|^2(x) \leq 2 [P_t(u_0 \log u_0)(x) - P_t(u_0)(x) \log P_t(u_0)(x)],$$

*from which we derive (1.5). However, our method is useful to study estimates for other (nonlinear) PDEs with subelliptic operators, see Theorems 3.8 and 3.9 in Section 3.*

**Remark 1.3** *Theorem 1.1 is very closed to Harnack estimate for the heat equation which is dimension free, see R. Hamilton [13]. The relation between the Bakry-Ledoux reverse logarithmic Sobolev inequality and a slight improvement of Hamilton's Harnack inequality was discussed in a very interesting paper by X. D. Li [21].*

Indeed we will establish a similar estimate for the heat equation with a sub-elliptic operator, under similar curvature conditions, and indeed we will establish a gradient estimate for a complete manifold whose Ricci curvature is bounded from below.

**Theorem 1.4** *Let  $M$  be a complete manifold of dimension  $n$  with non-negative Ricci curvature. Suppose  $u$  is non-negative solution to the heat equation of (1.3) with initial data  $u_0 > 0$ . If  $C \in [0, \infty]$  such that  $-\Delta \log u_0 \leq C$ , then*

$$|\nabla \log u|^2 - 2 \frac{\partial}{\partial t} \log u \leq \frac{C}{\frac{t}{n}C + 1} \quad \text{for } t \geq 0.$$

By setting  $C = \infty$  we recover Li-Yau's estimate (1.4).

The novelty of the present paper is not so much about the gradient estimates in Theorem 1.1 and Theorem 1.4, what is interesting of the present work is the approach we are going to develop in order to discover and prove these gradient estimates. Our approach brings together with the martingale analysis to the study of a class of non-linear PDEs with quadratic growth. Of course the connection between the harmonic analysis, potential theory and martingales is not new, which indeed has a long tradition, standard books may be mentioned in this aspect, such as [9], [10], [11] and etc., what is new in our study is an interesting connection between the BMO martingales and positive solutions of the heat equation (1.3).

To take into account of the positivity, it is better to consider the Hopf transformation of a positive solution  $u$  to (1.3), i.e.  $f = \log u$ , then  $f$  itself solves a parabolic equation with quadratic non-linear term, namely

$$\left(\frac{1}{2}\Delta - \frac{\partial}{\partial t}\right)f = -\frac{1}{2}|\nabla f|^2 \quad \text{in } [0, \infty) \times M. \quad (1.6)$$

The preceding equation (1.6) is an archetypical example of a kind of semi-linear parabolic equations with quadratic growth which has attracted much attention recently associated with backward stochastic differential equations, for example Kobylanski [17], Briand-Hu [6], Delbaen et al. [7] and etc.

The main idea may be described as the following. Suppose  $f$  is a smooth solution of the non-linear equation (1.6), and  $X_t = B_t + x$  where  $B$  is a standard Brownian motion on a complete probability space. Let  $Y_t = f(T - t, X_t)$  and  $Z_t = (Z_t^i)$  where  $Z_t^i = \nabla^i f(T - t, X_t)$ ,  $\nabla^i$  is the covariant derivative written in a local orthonormal coordinate system. Then, Itô's lemma applying to  $f$  and  $X$  may be written as

$$Y_T - Y_t = \sum_{i=1}^n \int_t^T Z_s^i dB_s^i - \frac{1}{2} \int_t^T |Z_s|^2 ds. \quad (1.7)$$

On the other hand, it was a remarkable discovery by Bismut [4] (for a special linear case) and Pardoux-Peng [25] that given the terminal random variable  $Y_T \in L^2(\Omega, \mathcal{F}_T, \mathbb{P})$ , there is actually a unique pair  $(Y, Z)$  where  $Y$  is a continuous semimartingale and  $Z$  is a predictable process which satisfies (1.7). The actual knowledge that  $Z$  is the gradient of  $Y$  may be restored if  $Y_T = f_0(X_T)$ . The backward stochastic differential equation (1.7) with a bounded random terminal  $Y_T$ , which has a non-linear term of quadratic growth and thus is not covered by Pardoux-Peng [25], was resolved by Kobylanski [17]. Observe that the martingale part of  $Y$  is the Itô integral of  $Z$  against Brownian motion  $B$  (which is denoted by  $Z.B$ ). It can be shown that, if  $Y$  is bounded, then  $Z.B$  is a BMO martingale up to time  $T$ , so that the exponential martingale

$$\mathcal{E}(h(Z).B)_t = \exp \left[ \sum_{i=1}^n \int_0^t h^i(Z_s) dB_s^i - \frac{1}{2} \int_0^t |h(Z_s)|^2 ds \right]$$

is a uniformly integrable martingale (up to time  $T$ ), as long as  $h$  is global Lipschitz continuous. The main technical step in our approach is that, due to the special feature of our non-linear term in (1.6), we can choose  $h^i(z) = z^i$  (one has to go through the detailed computations below to see why this choice of  $h^i$  is a good one), and making change of probability measure to  $\mathbb{Q}$  by  $\frac{d\mathbb{Q}}{d\mathbb{P}} = \mathcal{E}(h(Z).B)_T$ ,

then, under  $\mathbb{Q}$ , not only  $Z\tilde{B}$  is again a BMO martingale (where  $\tilde{B}$  is the martingale part of  $B$  under the new probability  $\mathbb{Q}$ ), but also  $t \rightarrow |Z_t|^2$  is a non-negative submartingale. Next by utilizing the BSDE (1.7), we can see the BMO norm of  $Z\tilde{B}$  under  $\mathbb{Q}$  is dominated at most  $2\sqrt{\|Y\|_\infty}$ , that is

$$\mathbb{E}^{\mathbb{Q}} \left\{ \int_t^T |Z_s|^2 ds \middle| \mathcal{F}_t \right\} \leq 4\|Y\|_\infty.$$

Finally the sub-martingale property of  $|Z_t|^2$  allows to move  $|Z_s|^2$  (for  $s \in (t, T)$ ) out from the time integral on the left-hand side of the previous inequality, which in turn yields the gradient estimate.

Let us now give a heuristic probabilistic proof to Theorem 1.4 to explain from where such estimates come from. Let  $f = \log u$ , and  $G = -\Delta f$ . Then one can show that

$$G = |\nabla f|^2 - 2f_t$$

(where  $f_t$  stands for the time derivative  $\frac{\partial}{\partial t}f$  for simplicity). Moreover,  $G$  satisfies

$$(L - \frac{\partial}{\partial t})G = \frac{1}{n}G^2 + H,$$

where

$$H = (|\nabla \nabla f|^2 - \frac{1}{n}G^2) + 2\text{Ric}(\nabla f, \nabla f),$$

and  $H \geq 0$ . We suppose here  $G > 0$ . Consider the BSDE:

$$dY_t = Z_t dB_t + \frac{1}{n}Y_t^2 dt, \quad Y_T = G(0, x + B_T).$$

Then

$$Y_t \geq G(T - t, x + B_t).$$

Setting

$$U_t = \frac{1}{Y_t}, \quad V_t = -\frac{Z_t}{Y_t^2},$$

then  $(U, V)$  satisfies the following quadratic BSDE:

$$dU_t = -\frac{1}{n}dt + V_t dB_t + \frac{|V_t|^2}{U_t}dt.$$

Using BMO martingale techniques, one can prove that there exists a new probability measure  $\mathbb{Q}$  under which  $\tilde{B}_t = B_t + \int_0^t \frac{V_s}{U_s} ds$  is a Brownian motion. Hence

$$dU_t = -\frac{1}{n}dt + V_t d\tilde{B}_t,$$

from which we deduce that  $U_0 = \frac{T}{n} + \mathbb{E}^{\mathbb{Q}}[U_T]$ , and

$$Y_0 = \frac{1}{\frac{T}{n} + \mathbb{E}^{\mathbb{Q}} \left[ \frac{1}{Y_T} \right]}$$

which yields the estimate in Theorem 1.4.

Even though the above heuristic proof is probabilistic (which can be made rigorous), we prefer to give a pure analytic proof in the last section.

The paper is organized as follows. Next section is devoted to some basic facts about quadratic BSDEs including BMO martingales. Section 3 establishes the gradient estimates for some linear parabolic PDEs on Euclidean space, while Section 4 establishes these estimates on complete manifold. Last section is devoted to establish a generalized Li-Yau estimate via analytic tool.

## 2 BSDE and BMO martingales

Let us begin with an interesting result about BSDEs with quadratic growth. The kind of BSDEs we will deal with in this paper has the following form

$$dY = \sum_{j=1}^m Z^j F^j(Y, Z) dt + \sum_{j=1}^m Z^j dB^j, \quad Y_T = \xi, \quad (2.1)$$

with terminal value  $\xi \in L^\infty(\Omega, \mathcal{F}_T, \mathbb{P})$  which is given, where  $B = (B^1, \dots, B^m)$  is a standard Brownian motion,  $(\mathcal{F}_t)_{t \geq 0}$  is the Brownian filtration associated with  $B$ , and  $F^j$  are continuous function on  $\mathbb{R} \times \mathbb{R}^m$  with at most linear growth: there is a constant  $C_1 \geq 0$  such that

$$|F(y, z)| \leq C_1(1 + |y| + |z|) \quad \forall (y, z) \in \mathbb{R} \times \mathbb{R}^m.$$

According to Peng [26] and as we have seen in the Introduction, if  $u$  is a bounded smooth solution to the following non-linear parabolic equation

$$\frac{\partial}{\partial t} u + \sum_{j=1}^d F^j(u, \nabla u) \frac{\partial u}{\partial x_j} = \frac{1}{2} \Delta u \quad \text{in } [0, \infty) \times \mathbb{R}^m, \quad (2.2)$$

with initial data  $u_0$ , then  $Y_t = u(T - t, B_t + \cdot)$  and  $Z_t = \nabla u(T - t, B_t + \cdot)$  is a solution pair of (2.1) with terminal value  $Y_T = u_0(B_T + \cdot)$ . The special feature of (2.2) is that the maximum principle applies, which implies that global solutions (here global means for large  $t$ ) exist for the initial value problem of the system as long as the initial data is bounded (though, this constraint can be relaxed a bit, but for the simplicity we content ourself to the bounded initial data problem). The maximum principle implies that as long as  $u$  is a solution to (2.2) then  $|u(x, t)| \leq \|u_0\|_\infty$ . Therefore, if the initial data  $u_0$  is bounded, and  $F^j$  are global Lipschitz, then, according to Theorem 6.1 on page 592, [19],  $u$  exists for all time, and both  $u$  and  $\nabla u$  are bounded on  $\mathbb{R}^m \times [0, T]$ .

The maximum principle for (2.1) however remains true even for a bounded random terminal value (so called non Markovian case), which in turn yields that the martingale part of  $Y$  is a BMO martingale. This is the context of the following

**Proposition 2.1** *Suppose that  $\xi \in L^\infty(\Omega, \mathcal{F}_T, \mathbb{P})$ . There exists a unique solution  $(Y, Z)$  to (2.1) such that  $Y$  is bounded and  $M = Z \cdot B$  is a square integrable martingale. Moreover  $M = Z \cdot B$  is a BMO martingale up to time  $T$ , and*

$$\|Y(t)\|_\infty \leq \|\xi\|_\infty \quad \forall t \in [0, T].$$

**Proof.** The existence and uniqueness is already given in [17]. The fact that  $M = Z.B$  is a BMO martingale up to time  $T$  is proved in [24]. Then there exists a constant  $C_2 > 0$  such that

$$\mathbb{E} \left[ \int_t^T |Z_s|^2 ds \middle| \mathcal{F}_t \right] \leq C_2.$$

Let  $N_t = \sum_{j=1}^d \int_0^t F^j(Y_s, Z_s) dB_s^j$ . Since

$$\begin{aligned} \langle N, N \rangle_T - \langle N, N \rangle_t &= \int_t^T \sum_j |F^j(Y_s, Z_s)|^2 ds \\ &\leq \int_t^T C_1^2 (1 + |Y_s| + |Z_s|)^2 ds, \end{aligned}$$

so there exists a constant  $C_3 > 0$  such that

$$\mathbb{E} \{ \langle N, N \rangle_T - \langle N, N \rangle_t \middle| \mathcal{F}_t \} \leq C_3.$$

Therefore  $N$  is a BMO martingale. Hence the stochastic exponential  $\mathcal{E}(-N)$  is a martingale up to  $T$ .

Define a probability measure  $\mathbb{Q}$  on  $(\Omega, \mathcal{F}_T)$  by  $d\mathbb{Q}/d\mathbb{P} = \mathcal{E}(-N)_T$ . Then, according to Girsanov's theorem  $\tilde{B}_t = B_t + \langle N, B \rangle_t$  is a Brownian motion up to time  $T$  under  $\mathbb{Q}$ , and  $(Y, Z)$  is a solution to the simple BSDE

$$dY_t = Z_t d\tilde{B}_t$$

under the probability  $\mathbb{Q}$ , whose solution is given by

$$Y_t = \mathbb{E}^{\mathbb{Q}} \{ \xi \middle| \mathcal{F}_t \} = \mathbb{E} \{ \mathcal{E}(-N)_T \mathcal{E}(-N)_t^{-1} \xi \middle| \mathcal{F}_t \} \quad \text{for } t \leq T. \quad (2.3)$$

It particularly implies that  $\|Y_t\|_{\infty} \leq \|\xi\|_{\infty}$ . ■

### 3 Stochastic flows and gradient estimates

Let  $A_0, A_1, \dots, A_m$  be  $m+1$  smooth vector fields on Euclidean space  $\mathbb{R}^n$ , where  $n$  is a non-negative integer. Then, we may form a sub-elliptic differential operator of second order in  $\mathbb{R}^n$ :

$$L = \frac{1}{2} \sum_{\alpha=1}^m A_{\alpha}^2 + A_0, \quad (3.1)$$

here we add a factor  $\frac{1}{2}$  in order to save the constant  $\sqrt{2}$  in front of Brownian motion which will appear frequently in computations in the remaining of the paper. Our goal is to devise an explicit gradient estimate for a (smooth) positive solution  $u$  of the heat equation

$$\left( L - \frac{\partial}{\partial t} \right) u = 0, \quad \text{on } (0, \infty) \times \mathbb{R}^n, \quad (3.2)$$

by utilizing the BSDE associated with the Hopf transformation  $f = \log u$ , which satisfies the semi-linear parabolic equation

$$\left( L - \frac{\partial}{\partial t} \right) f = -\frac{1}{2} \sum_{\alpha=1}^m |A_{\alpha} f|^2, \quad \text{on } (0, \infty) \times \mathbb{R}^n. \quad (3.3)$$

### 3.1 Stochastic flow

The first ingredient in our approach is the theory of stochastic flows defined by the following stochastic differential equation

$$d\varphi = A_0(\varphi)dt + \sum_{\alpha=1}^m A_\alpha(\varphi) \circ dw^\alpha, \quad \varphi(0, \cdot) = x, \quad (3.4)$$

where  $\circ d$  denotes the Stratonovich differential, developed by Baxendale [3], Bismut [5], Eells and Elworthy [12], Malliavin [23], Kunita [18] and etc. The reader may refer to Ikeda and Watanabe [15] for a definite account. To ensure the global existence of a stochastic flow, we require the following condition to be satisfied.

**Condition 3.1** *Let  $A_\alpha = \sum_{j=1}^n A_\alpha^j \frac{\partial}{\partial x^j}$ . Assume that  $A_\alpha^j$  have bounded derivatives.*

By writing (3.4) in terms of Itô's stochastic integrals, namely

$$d\varphi^j = \left[ A_0^j + \frac{1}{2} \sum_{\alpha=1}^m A_\alpha^i \frac{\partial A_\alpha^j}{\partial x^i} \right] (\varphi) dt + \sum_{\alpha=1}^m A_\alpha^j(\varphi) dw^\alpha, \quad \varphi(0, \cdot) = x, \quad (3.5)$$

where (and thereafter) Einstein's summation convention has been used: repeated indices such as  $i$  is summed up from 1 up to  $n$ . The existence and uniqueness of a strong solution follow directly from the standard result in Itô's theory, which in turn determines a diffusion process in  $\mathbb{R}^n$  with the infinitesimal generator  $L$ .

In fact, more can be said about the unique strong solution, and important consequences are collected here which will be used later on. Suppose  $w = (w_t)$  is a standard Brownian motion (started at 0) with its Brownian filtration  $(\mathcal{F}_t)_{t \geq 0}$  on the classical Wiener space  $(\Omega, \mathcal{F}, \mathbb{P})$  of dimension  $m$ , so that  $w = (w_t)_{t \geq 0}$  is the coordinate process on the space  $\Omega$  of continuous paths in  $\mathbb{R}^m$  with initial zero. Then, there is a measurable mapping  $\varphi : \mathbb{R}^+ \times \Omega \times \mathbb{R}^n \rightarrow \mathbb{R}^n$  and a probability null set  $\mathcal{N}$ , which possess the following properties.

1.  $w \rightarrow \varphi(t, w, x)$  is  $\mathcal{F}_t$ -measurable for  $t \geq 0$  and  $x \in \mathbb{R}^n$ , and  $\varphi(0, w, x) = x$  for every  $w \in \Omega \setminus \mathcal{N}$  and  $x \in \mathbb{R}^n$ .
2.  $t \rightarrow \varphi(t, w, x)$  is continuous, that is  $\varphi(\cdot, w, x) \in C(\mathbb{R}^+, \mathbb{R}^n)$ , for  $w \in \Omega \setminus \mathcal{N}$  and  $x \in \mathbb{R}^n$ .  $t \rightarrow \varphi(t, \cdot, x)$  is a continuous semimartingale for any  $x \in \mathbb{R}^n$ .
3.  $x \rightarrow \varphi(t, w, x)$  is a diffeomorphism of  $\mathbb{R}^n$  for each  $w \in \Omega \setminus \mathcal{N}$  and  $t \geq 0$ . That is  $x \rightarrow \varphi(t, w, x)$  is smooth and its inverse exists, and the inverse is also smooth.
4. The family  $\{\varphi(t, \cdot, x) : t \geq 0, x \in \mathbb{R}^n\}$  is a stochastic flow:

$$\varphi(t+s, w, x) = \varphi(t, \theta_s w, \varphi(s, w, x))$$

for all  $t, s \geq 0$ ,  $x \in \mathbb{R}^n$  and  $w \in \Omega \setminus \mathcal{N}$ , where  $\theta_s : \Omega \rightarrow \Omega$  is the shift operator sending a path  $w$  to a path  $\theta_s w(t) = w(t+s)$  for  $t \geq 0$ .

5. For each  $x \in \mathbb{R}^n$ ,  $\varphi(t) = \varphi(t, \cdot, x)$  (or denoted by  $\varphi(t, x)$ ) is the unique strong solution of (3.4).



6. Let  $J_j^i(t, w, x) = \frac{\partial \varphi^i(t, w, x)}{\partial x^j}$  for  $i, j \leq n$ . Then  $J_j^i(0, w, x) = \delta_j^i$  and  $J$  solves the following SDE

$$dJ_j^i = \frac{\partial A_0^i}{\partial x^l}(\varphi) J_j^l dt + \sum_{\alpha=1}^m \frac{\partial A_\alpha^i}{\partial x^l}(\varphi) J_j^l \circ dw^\alpha, \quad J_j^i(0) = \delta_j^i, \quad (3.6)$$

and its inverse matrix  $K = J^{-1} = (K_j^i)$  solves

$$dK_j^i = -K_l^i \frac{\partial A_0^l}{\partial x^j}(\varphi) dt - \sum_{\alpha=1}^m K_l^i \frac{\partial A_\alpha^l}{\partial x^j}(\varphi) \circ dw^\alpha, \quad K_j^i(0) = \delta_j^i. \quad (3.7)$$

In our computations below, we have to use Itô's integrals rather than Stratonovich's ones. Therefore we would like to rewrite (3.6, 3.7) in terms of Itô's differential, so

$$\begin{aligned} dJ_j^i &= \sum_{\alpha=1}^m \frac{\partial A_\alpha^i}{\partial x^l}(\varphi) J_j^l dw^\alpha \\ &+ \left[ \frac{\partial A_0^i}{\partial x^l} + \frac{1}{2} \sum_{\alpha=1}^m \left( A_\alpha^k \frac{\partial^2 A_\alpha^i}{\partial x^l \partial x^k} + \frac{\partial A_\alpha^k}{\partial x^l} \frac{\partial A_\alpha^i}{\partial x^k} \right) \right] (\varphi) J_j^l dt, \end{aligned} \quad (3.8)$$

and

$$\begin{aligned} dK_j^i &= - \sum_{\alpha=1}^m K_l^i \frac{\partial A_\alpha^l}{\partial x^j}(\varphi) dw^\alpha \\ &- K_l^i \left[ \frac{\partial A_0^l}{\partial x^j} + \frac{1}{2} \sum_{\alpha=1}^m \left( A_\alpha^k \frac{\partial^2 A_\alpha^l}{\partial x^j \partial x^k} - \frac{\partial A_\alpha^k}{\partial x^j} \frac{\partial A_\alpha^l}{\partial x^k} \right) \right] (\varphi) dt. \end{aligned} \quad (3.9)$$

### 3.2 Structure assumptions

We introduce some technical assumptions on the structure of the Lie algebra generated by the family of vector fields  $\{A_0, A_1, \dots, A_m\}$ , in addition to Condition 3.1. Recall that  $A_\alpha = A_\alpha^j \frac{\partial}{\partial x^j}$ , and  $A_{\alpha,\beta}^j, A_{\alpha,\beta,\gamma}^j$  etc. are the corresponding coefficients in Lie brackets

$$[A_\alpha, A_\beta] = A_{\alpha,\beta}^j \frac{\partial}{\partial x^j}, \quad [A_\alpha, [A_\beta, A_\gamma]] = A_{\alpha,\beta,\gamma}^j \frac{\partial}{\partial x^j} \text{ etc.},$$

where

$$\begin{aligned} A_{\alpha,\beta}^j &= A_\alpha^i \frac{\partial A_\beta^j}{\partial x^i} - A_\beta^i \frac{\partial A_\alpha^j}{\partial x^i}, \\ A_{\beta,\beta,\alpha}^k &= A_\beta^j A_\beta^i \frac{\partial^2 A_\alpha^k}{\partial x^i \partial x^j} - A_\beta^j A_\alpha^i \frac{\partial^2 A_\beta^k}{\partial x^i \partial x^j} + A_\beta^i \frac{\partial A_\alpha^k}{\partial x^j} \frac{\partial A_\beta^j}{\partial x^i} \\ &- 2A_\beta^j \frac{\partial A_\alpha^i}{\partial x^j} \frac{\partial A_\beta^k}{\partial x^i} + A_\alpha^i \frac{\partial A_\beta^j}{\partial x^i} \frac{\partial A_\beta^k}{\partial x^j}. \end{aligned} \quad (3.10)$$

etc. Let

$$R_\alpha^k = \sum_{\beta=1}^m A_{\beta,\beta,\alpha}^k = \sum_{\beta=1}^m [A_\beta, [A_\beta, A_\alpha]]^k. \quad (3.11)$$

**Condition 3.2** *There is a constant  $C_1 \geq 0$  such that for any  $\xi = (\xi_i)_{i \leq n}$ ,  $\theta_\beta = (\theta_{i,\beta})_{i \leq n} \in \mathbb{R}^n$  ( $\beta = 1, \dots, m$ ), it holds that*

$$\begin{aligned} & \sum_{\alpha,\beta=1}^m \left( \sum_{k=1}^n A_\alpha^k \theta_{k,\beta} \right)^2 + 2 \sum_{\alpha,\beta=1}^m \left( \sum_{k=1}^n \xi_k A_{\beta,\alpha}^k \right) \left( \sum_{i=1}^n A_\alpha^i \theta_{i,\beta} \right) \\ & + 2 \sum_{\alpha,\beta=1}^m \left( \sum_{k=1}^n \xi_k A_\alpha^k \right) \left( \sum_{i=1}^n A_{\beta,\alpha}^i \theta_{i,\beta} \right) \\ & \geq -C_1 \sum_{\alpha=1}^m \left( \sum_{k=1}^n A_\alpha^k \xi_k \right)^2 \end{aligned}$$

i.e.

$$\begin{aligned} & \sum_{\alpha,\beta=1}^m (\langle A_\alpha, \theta_\beta \rangle^2 + 2\langle A_\alpha, \xi \rangle \langle A_{\beta,\alpha}, \theta_\beta \rangle + 2\langle A_\alpha, \theta_\beta \rangle \langle A_{\beta,\alpha}, \xi \rangle) \\ & \geq -C_1 \sum_{\alpha=1}^m \langle A_\alpha, \xi \rangle^2. \end{aligned}$$

**Condition 3.3** *There is a constant  $C_2 \geq 0$  such that for any  $\xi = (\xi_i)_{i \leq n} \in \mathbb{R}^n$*

$$\begin{aligned} & \sum_{i,k=1}^n \xi_i \left( \sum_{\alpha=1}^m (A_\alpha^i R_\alpha^k + 2A_\alpha^i A_{0,\alpha}^k) + \sum_{\alpha,\beta=1}^m A_{\beta,\alpha}^i A_{\beta,\alpha}^k \right) \xi_k \\ & \geq -C_2 \sum_{\alpha=1}^m \left( \sum_{k=1}^n A_\alpha^k \xi_k \right)^2. \end{aligned}$$

**Remark 3.4** *Condition (3.1) is standard in the literature, while Conditions (3.2) and (3.3) are satisfied if  $A$  is elliptic or  $A$  satisfies the Frobenius integrability condition.*

Let us suppose the following Frobenius integrability condition: there exist some bounded smooth coefficients  $c_{\beta,\alpha}^l(x)$ , such that

$$A_{\beta,\alpha} = \sum_{l=1}^m c_{\beta,\alpha}^l A_l, \quad \beta = 0, 1, \dots, m, \quad \alpha = 1, \dots, m.$$

In other words, the Lie brackets  $A_{\beta,\alpha}$ ,  $\beta = 0, 1, \dots, m$ ,  $\alpha = 1, \dots, m$ , must lie in the linear span of  $A_1, \dots, A_m$ . Then the conditions (3.2) and (3.3) are satisfied.

Indeed,

$$\begin{aligned} [A_\beta, [A_\beta, A_\alpha]]^j &= A_\beta^i \frac{\partial}{\partial x^i} (c_{\beta,\alpha}^l A_l^j) - c_{\beta,\alpha}^l A_l^i \frac{\partial A_\beta^j}{\partial x^i} \\ &= c_{\beta,\alpha}^l A_{\beta,l}^j + \frac{\partial c_{\beta,\alpha}^l}{\partial x^i} A_\beta^i A_l^j \\ &= (c_{\beta,\alpha}^l c_{\beta,l}^k + \frac{\partial c_{\beta,\alpha}^k}{\partial x^i} A_\beta^i) A_k^j. \end{aligned}$$

This means that  $[A_\beta, [A_\beta, A_\alpha]]$  also lies in the linear span of  $A_1, \dots, A_m$ , and the conditions (3.2) and (3.3) are easily checked.

### 3.3 The density processes $Z_\alpha$

Let us consider a smooth solution  $f$  to the following non-linear parabolic equation

$$\left(L - \frac{\partial}{\partial t}\right) f = h(f, A_\alpha f), \quad \text{on } \mathbb{R}_+ \times \mathbb{R}^n, \quad (3.12)$$

where  $h$  is a  $C^1$ -function on  $\mathbb{R} \times \mathbb{R}^m$ , though our archetypical example is  $f = \log u$  and  $u$  is a positive solution to equation (3.3).

By Itô's formula,

$$Y_t = Y_T - \sum_{\alpha=1}^m \int_t^T Z^\alpha dw^\alpha - \int_t^T h(Y, Z) ds, \quad (3.13)$$

where

$$\begin{aligned} Y(t, w, x) &= f(T - t, \varphi(t, w, x)), \\ Z^\alpha(t, w, x) &= (A_\alpha f)(T - t, \varphi(t, w, x)) \end{aligned}$$

for  $\alpha = 1, \dots, m$ , and  $Z = (Z^\alpha)$ . The arguments  $w$  and  $/$  or  $x$  will be suppressed if no confusion may arise. Equivalently

$$dY = \sum_{\alpha=1}^m Z^\alpha dw^\alpha + h(Y, Z) dt. \quad (3.14)$$

Our aim in this part is to show that  $Z$  is an Itô process, and derives stochastic differential equations for  $Z$  (which in turn gives its Doob-Meyer's decomposition).

It is clear that both  $Y$  and  $Z^\alpha$  ( $\alpha = 1, \dots, m$ ) are continuous semimartingales. Taking derivatives with respect to  $x^i$  ( $i = 1, \dots, n$ ) in the equation (3.14) one obtains

$$dY_i = \sum_{\alpha=1}^m Z_i^\alpha dw^\alpha + \left( h_y(Y, Z) Y_i + \sum_{\alpha=1}^m h_{z_\alpha}(Y, Z) Z_i^\alpha \right) dt, \quad (3.15)$$

where

$$Y_i = \frac{\partial}{\partial x^i} Y \quad \text{and} \quad Z_i^\alpha = \frac{\partial}{\partial x^i} Z^\alpha, \quad i = 1, \dots, n,$$

and

$$h_y = \frac{\partial}{\partial y} h(y, z), \quad h_{z_\alpha} = \frac{\partial}{\partial z_\alpha} h(y, z), \quad \alpha = 1, \dots, m.$$

On the other hand, by definition,

$$Y_i(t, \cdot, x) = \frac{\partial}{\partial x^i} Y(t, \cdot, x) = \frac{\partial f}{\partial \varphi^j}(t, \varphi(t, \cdot, x)) J_i^j(t, \cdot, x),$$

so

$$\frac{\partial f}{\partial \varphi^k}(t, \varphi(t, \cdot, x)) = K_k^l(t, \cdot, x) Y_l(t, \cdot, x).$$

It follows that

$$\begin{aligned} Z^\alpha(t, \cdot, x) &= A_\alpha^k(\varphi(t, \cdot, x)) \frac{\partial f}{\partial \varphi^k}(\varphi(t, \cdot, x)) \\ &= A_\alpha^k(\varphi(t, \cdot, x)) K_k^l(t, \cdot, x) Y_l(t, \cdot, x), \end{aligned} \quad (3.16)$$

which implies that  $Z$  is a continuous semimartingale. The equation (3.16) is not new, and has been used by many authors in different contexts.

We next would like to write down the stochastic differential equations that  $Z^\alpha$  must satisfy by using the relation (3.16), which is however an easy exercise on integration by parts. Indeed, we have

$$\begin{aligned} dZ^\alpha &= Y_l K_k^l \frac{\partial A_\alpha^k}{\partial x^j}(\varphi) d\varphi^j + Y_l A_\alpha^k(\varphi) dK_k^l + A_\alpha^k(\varphi) K_k^l dY_l \\ &\quad + Y_l \frac{\partial A_\alpha^k}{\partial x^j}(\varphi) d\langle \varphi^j, K_k^l \rangle + K_k^l \frac{\partial A_\alpha^k}{\partial x^j}(\varphi) d\langle \varphi^j, Y_l \rangle \\ &\quad + A_\alpha^k(\varphi) d\langle K_k^l, Y_l \rangle + \frac{1}{2} Y_l K_k^l \frac{\partial^2 A_\alpha^k}{\partial x^i \partial x^j}(\varphi) d\langle \varphi^i, \varphi^j \rangle. \end{aligned} \quad (3.17)$$

Using the SDEs (3.4, 3.9) and the BSDE (3.15), through a lengthy but completely elementary computation, we establish the following Doob-Meyer's decomposition for  $Z$

$$\begin{aligned} dZ^\alpha &= \sum_{\beta=1}^m U_{\alpha,\beta} \left( dw^\beta + h_{z_\beta}(Y, Z) dt \right) + K_k^l \sum_{\beta=1}^m A_{\beta,\alpha}^k Z_l^\beta dt \\ &\quad + K_k^l Y_l \left[ A_{0,\alpha}^k + \frac{1}{2} \sum_{\beta=1}^m A_{\beta,\beta,\alpha}^k + A_\alpha^k h_y(Y, Z) - \sum_{\beta=1}^m A_{\beta,\alpha}^k h_{z_\beta}(Y, Z) \right] dt, \end{aligned} \quad (3.18)$$

where repeated indices are added up from 1 to  $n$ ,

$$U_{\alpha,\beta} = K_k^l \left( A_{\beta,\alpha}^k Y_l + A_\alpha^k Z_l^\beta \right) \quad (3.19)$$

and

$$A_{\beta,\alpha}^k = [A_\beta, A_\alpha]^k, \quad A_{\beta,\beta,\alpha}^k = [A_\beta, [A_\beta, A_\alpha]]^k.$$

We are now in a position to work out the Doob-Meyer's decomposition for

$$|Z|^2 = \sum_{\alpha=1}^m |Z^\alpha|^2$$

which simply follows from Itô's formula and (3.18). In order to simplify our displayed formula, we introduce the following notations:

$$\xi_i = \sum_{j=1}^n K_i^j Y_j, \quad \theta_{k,\beta} = \sum_{j=1}^n K_k^j Z_j^\beta,$$

for  $i, k = 1, \dots, n$  and  $\beta = 1, \dots, m$ , so that

$$Z^\alpha = \sum_{j=1}^n A_\alpha^j \xi_j \quad \text{and} \quad |Z|^2 = \sum_{\alpha=1}^m \left( \sum_{j=1}^n A_\alpha^j \xi_j \right)^2. \quad (3.20)$$

Let

$$d\tilde{w}^\beta = dw^\beta + h_{z_\beta}(Y, Z)dt,$$

which is a Brownian motion under probability  $\mathbb{Q}$  with the Cameron-Martin density

$$\left. \frac{d\mathbb{Q}}{d\mathbb{P}} \right|_{\mathcal{F}_t} = \exp \left[ - \sum_{\beta=1}^m \int_0^t h_{z_\beta}(Y, Z) dw^\beta - \frac{1}{2} \int_0^t \sum_{\beta=1}^m |h_{z_\beta}(Y, Z)|^2 ds \right]. \quad (3.21)$$

Then, by an elementary computation,

$$\begin{aligned} d|Z|^2 &= 2 \sum_{\alpha, \beta=1}^m \left( Z^\alpha \xi_k A_{\beta, \alpha}^k + \xi_i A_\alpha^i A_\alpha^k \theta_{k, \beta} \right) d\tilde{w}^\beta \\ &+ \left[ \sum_{\alpha, \beta=1}^m A_\alpha^k \theta_{k, \beta} A_\alpha^i \theta_{i, \beta} + 2\xi_k \sum_{\alpha, \beta=1}^m \left( A_{\beta, \alpha}^k A_\alpha^i + A_{\beta, \alpha}^i A_\alpha^k \right) \theta_{i, \beta} \right] dt \\ &+ 2 \left[ h_y(Y, Z) \sum_{\alpha=1}^m A_\alpha^i A_\alpha^k - \sum_{\alpha, \beta=1}^m A_\alpha^i A_{\beta, \alpha}^k h_{z_\beta}(Y, Z) \right] \xi_i \xi_k dt \\ &+ \left[ \sum_{\alpha=1}^m A_\alpha^i \left( R_\alpha^k + 2A_{0, \alpha}^k \right) + \sum_{\alpha, \beta=1}^m A_{\beta, \alpha}^i A_{\beta, \alpha}^k \right] \xi_i \xi_k dt. \end{aligned} \quad (3.22)$$

**Lemma 3.5** *If  $h(Y, Z) = h(Y, |Z|^2)$ , then*

$$\begin{aligned} d|Z|^2 &= 2 \sum_{\alpha, \beta=1}^m \left( Z^\alpha \xi_k A_{\beta, \alpha}^k + \xi_i A_\alpha^i A_\alpha^k \theta_{k, \beta} \right) d\tilde{w}^\beta \\ &+ \left[ \sum_{\alpha, \beta=1}^m A_\alpha^k \theta_{k, \beta} A_\alpha^i \theta_{i, \beta} + 2\xi_k \sum_{\alpha, \beta=1}^m \left( A_{\beta, \alpha}^k A_\alpha^i + A_{\beta, \alpha}^i A_\alpha^k \right) \theta_{i, \beta} \right] dt \\ &+ \left[ \sum_{\alpha=1}^m A_\alpha^i \left( R_\alpha^k + 2A_{0, \alpha}^k + 2A_\alpha^k h_y(Y, |Z|^2) \right) + \sum_{\alpha, \beta=1}^m A_{\beta, \alpha}^i A_{\beta, \alpha}^k \right] \xi_i \xi_k dt. \end{aligned} \quad (3.23)$$

**Proof.** In this case

$$\begin{aligned} \sum_{i, k, \alpha, \beta} \xi_i A_\alpha^i A_{\beta, \alpha}^k h_{z_\beta}(Y, Z) \xi_k &= 2 \sum_{i, k, \alpha, \beta} h' \xi_i A_\alpha^i A_{\beta, \alpha}^k A_\beta^l \xi_l \xi_k \\ &= -2 \sum_{i, k, \alpha, \beta} h' \xi_l A_\beta^l A_{\beta, \alpha}^k A_\alpha^i \xi_i \xi_k, \end{aligned}$$

so

$$\sum_{i, k, \alpha, \beta} \xi_i A_\alpha^i A_{\beta, \alpha}^k h_{z_\beta}(Y, Z) \xi_k = 0,$$

and thus (3.23) follows directly from (3.22). ■

### 3.4 Gradient estimates

Recall that  $f$  is a smooth solution to the non-linear parabolic equation (3.12), where the nonlinear term  $h(Y, Z)$  has at most quadratic growth. In order to devise explicit estimate for  $A_\alpha f$  ( $\alpha = 1, \dots, m$ ), we assume the following condition to be satisfied.

**Condition 3.6**  $h(y, z)$  depends only on  $(y, |z|^2)$ , i.e. there is a continuously differentiable function denoted again by  $h$  so that  $h(y, z) = h(y, |z|^2)$ , and we assume that

$$\frac{\partial}{\partial y} h(y, z) \geq 0.$$

Then, under Conditions (3.1, 3.2, 3.3, 3.6), according to (3.23), we have

$$d|Z|^2 \geq -K|Z|^2 dt + 2 \left( Z^\alpha \xi_k A_{\beta, \alpha}^k + \xi_i A_\alpha^i A_{\alpha, \beta}^k \theta_{k, \beta} \right) d\tilde{w}^\beta, \quad (3.24)$$

where  $K = C_1 + C_2$ .

**Lemma 3.7** Assume that Conditions (3.1, 3.2, 3.3, 3.6) are satisfied. Then  $M_t = e^{Kt}|Z_t|^2$  is submartingale under the probability  $\mathbb{Q}$  (up to terminal time  $T$ ):

$$\mathbb{E}^{\mathbb{Q}} \{M_t | \mathcal{F}_s\} \geq M_s, \quad \forall 0 \leq s < t \leq T. \quad (3.25)$$

**Proof.** By Itô's formula

$$dM = KM dt + e^{Kt} d|Z|^2,$$

hence, for any  $0 \leq s \leq t \leq T$ , we have

$$\begin{aligned} M_t - M_s &= K \int_s^t M_r dr + \int_s^t e^{Kr} d|Z|^2 \\ &\geq 2 \int_s^t e^{Ks} \sum_{\alpha, \beta=1}^m \left( Z^\alpha \xi_k A_{\beta, \alpha}^k + \xi_i A_\alpha^i A_{\alpha, \beta}^k \theta_{k, \beta} \right) d\tilde{w}^\beta, \end{aligned}$$

which yields (3.25). ■

We are now in a position to prove the following gradient estimate.

**Theorem 3.8** Assume that Conditions (3.1, 3.2, 3.3) are satisfied. Then

$$\sum_{\alpha=1}^m |A_\alpha \log u(t, x)|^2 \leq \frac{4K}{1 - e^{-K(T-t)}} \|\log u_0\|_\infty, \quad (3.26)$$

for any positive solution  $u$  of (3.2).

**Proof.** Apply the computations in the preceding sub-section to  $f = \log u$ , and  $h(y, z) = -\frac{1}{2}|z|^2$ . Then, under the probability  $\mathbb{Q}$  (defined by (3.21))

$$Y_t = Y_T - \sum_{\alpha=1}^m \int_t^T Z^\alpha d\tilde{w}^\alpha + \int_t^T \left[ \sum_{\alpha=1}^m Z^\alpha h_{z_\alpha}(Y, Z) - h(Y, Z) \right] ds,$$

thus

$$Y_t = Y_T - \sum_{\alpha=1}^m \int_t^T Z^\alpha d\tilde{w}^\alpha - \frac{1}{2} \int_t^T |Z_s|^2 ds,$$

and therefore

$$\begin{aligned} \mathbb{E}^\mathbb{Q} \left\{ \frac{1}{2} \int_t^T |Z_s|^2 ds \middle| \mathcal{F}_t \right\} &= \mathbb{E}^\mathbb{Q} \{ Y_T - Y_t | \mathcal{F}_t \} \\ &\leq 2 \|Y_T\|_\infty \leq 2 \|\log u_0\|_\infty. \end{aligned} \quad (3.27)$$

On the other hand,  $M_t = e^{Kt}|Z_t|^2$  is a submartingale, thus one has

$$\mathbb{E}^\mathbb{Q} \{ |Z_s|^2 | \mathcal{F}_t \} \geq e^{K(t-s)} |Z_t|^2, \quad \forall s \in [t, T],$$

so

$$\begin{aligned} \mathbb{E}^\mathbb{Q} \left\{ \frac{1}{2} \int_t^T |Z_s|^2 ds \middle| \mathcal{F}_t \right\} &\geq \frac{1}{2} \int_t^T e^{K(t-s)} |Z_t|^2 ds \\ &= \frac{1 - e^{-K(T-t)}}{2K} |Z_t|^2. \end{aligned} \quad (3.28)$$

Putting (3.27, 3.28) together, we obtain

$$|Z_t|^2 \leq \frac{4K}{1 - e^{-K(T-t)}} \|\log u_0\|_\infty,$$

which yields (3.26). ■

In general, we may proceed with  $f = \psi(u)$  where  $\psi$  is a concave function, and  $u$  is a positive solution to (1.1), thus  $f$  solves (3.3) with

$$h(y, z) = \frac{1}{2} \frac{\psi''(\psi^{-1}(y))}{|\psi'^{-1}(y)|^2} |z|^2.$$

We can proceed as above. Under the probability  $\mathbb{Q}$

$$Y_t = Y_T - \sum_{\alpha=1}^m \int_t^T Z^\alpha d\tilde{w}^\alpha + \int_t^T \left[ \sum_{\alpha=1}^m Z^\alpha h_{z_\alpha}(Y, Z) - h(Y, Z) \right] ds,$$

so

$$Y_t = Y_T - \sum_{\alpha=1}^m \int_t^T Z^\alpha d\tilde{w}^\alpha + \frac{1}{2} \int_t^T \frac{\psi''(\psi^{-1}(Y_s))}{|\psi'^{-1}(Y_s)|^2} |Z_s|^2 ds.$$

It is important to note that if

$$\psi^{(3)}\psi' \leq 2|\psi''|^2,$$

then  $h_y(y, z) \geq 0$ , thus from Lemma 2.2 in [7],

$$\mathbb{E}^\mathbb{Q} \left\{ \int_t^T |Z_s|^2 ds \middle| \mathcal{F}_t \right\} \leq 4 \|Y_T\|_\infty^2 \leq 4 \|\log u_0\|_\infty^2. \quad (3.29)$$

On the other hand  $M_t = e^{Kt}|Z_t|^2$  is a submartingale, thus one has

$$\mathbb{E}^{\mathbb{Q}} \{ |Z_s|^2 \mid \mathcal{F}_t \} \geq e^{K(t-s)} |Z_t|^2, \quad \forall s \in [t, T],$$

and therefore

$$\begin{aligned} \mathbb{E}^{\mathbb{Q}} \left\{ \int_t^T |Z_s|^2 ds \mid \mathcal{F}_t \right\} &\geq \int_t^T e^{K(t-s)} |Z_t|^2 ds \\ &= \frac{1 - e^{-K(T-t)}}{K} |Z_t|^2. \end{aligned} \quad (3.30)$$

Putting (3.29, 3.30) together, we can obtain

$$|Z_t|^2 \leq \frac{4K}{1 - e^{-K(T-t)}} \|\log u_0\|_{\infty}^2,$$

which yields the following estimate.

**Theorem 3.9** *Assume that Conditions (3.1, 3.2, 3.3) are satisfied. Moreover,  $\psi$  is concave and satisfies:*

$$\psi^{(3)}\psi' \leq 2|\psi''|^2.$$

Then

$$\sum_{\alpha=1}^m |A_{\alpha}\psi(u(t, x))|^2 \leq \frac{4K}{1 - e^{-K(T-t)}} \|\psi(u_0)\|_{\infty}^2, \quad (3.31)$$

for any positive solution  $u$  of (3.2).

## 4 Heat equation on complete manifold

In this section, we study positive solutions of the heat equation

$$\left( \frac{1}{2}\Delta - \frac{\partial}{\partial t} \right) u = 0, \quad \text{in } [0, \infty) \times M, \quad (4.1)$$

where  $M$  is a complete manifold of dimension  $n$ ,  $\Delta$  is the Beltrami-Laplace operator. In a local coordinate system so that the Riemann metric  $ds^2 = g_{ij}dx^i dx^j$  and

$$\Delta = \frac{1}{\sqrt{g}} \sum_{i,j=1}^n \frac{\partial}{\partial x^i} g^{ij} \sqrt{g} \frac{\partial}{\partial x^j},$$

where  $g = \det(g_{ij})$  and  $(g^{ij})$  is the inverse matrix of  $(g_{ij})$ . We prove the following

**Theorem 4.1** *Suppose the Ricci curvature  $\text{Ric} \geq -K$  for some  $K \geq 0$ , and suppose  $u$  is a positive solution of (4.1) with initial data  $u_0 > 0$ . Then*

$$|\nabla \log u|^2(t, x) \leq \frac{2K}{1 - e^{-\frac{Kt}{2}}} \|\log u_0\|_{\infty}. \quad (4.2)$$



**Remark 4.2** *This estimate can also be derived from the reverse logarithmic Sobolev inequality, as in Remark 1.2.*

The preceding theorem is proved by using similar computations as in the proof of Theorem 3.7 but working on the orthonormal frame bundle  $O(M)$  over  $M$ .

Recall that a point  $\gamma = (x, e) \in O(M)$ , where  $(e_1, \dots, e_n)$  is an orthonormal basis of the tangent space  $T_x M$  at  $x \in M$ . Let  $\pi : \gamma = (x, e) \rightarrow x$  be the natural projection from  $O(M)$  to  $M$ .  $O(M)$  is a principal fibre bundle with its structure group  $O(n)$ . For the general facts on differential geometry, we refer to Kobayashi and Nomizu [16].

Suppose  $x = (x^1, \dots, x^n)$  is a local coordinate system on  $M$ , then it induces a local coordinate system  $\gamma = (x^k, e_j^i)$  on  $O(M)$  so that  $e_j = e_j^i \frac{\partial}{\partial x^i}$ . If  $L$  is a vector field, then  $\tilde{L}$  denotes the horizontal lifting of  $L$  to  $O(M)$ :

$$\tilde{L}(x, e) = L^i(x) \frac{\partial}{\partial x^i} - \Gamma(x)_{ij}^k L^i(x) e_l^j \frac{\partial}{\partial e_l^k}$$

in a local coordinate system, where  $\Gamma_{ij}^k$  are the Christoffel symbols associated with the Levi-Civita connection, and  $L = L^i \frac{\partial}{\partial x^i}$ . For  $\alpha = 1, \dots, n$  and  $\gamma = (x, e)$ , then  $\tilde{L}_\alpha$  denotes the horizontal lifting of  $e_\alpha$ , that is

$$\tilde{L}_\alpha(x, e) = e_\alpha^i \frac{\partial}{\partial x^i} - \Gamma(x)_{ij}^k e_\alpha^i e_l^j \frac{\partial}{\partial e_l^k}.$$

The system  $\{\tilde{L}_1, \dots, \tilde{L}_n\}$  is called the system of canonical horizontal vector fields. The mapping  $\tilde{L} : \mathbb{R}^n \rightarrow \Gamma(TO(M))$  where  $L_\xi = \xi^\alpha \tilde{L}_\alpha$ , is defined globally, and is independent of the choice of a local coordinate system. Therefore

$$\Delta_{O(M)} = \sum_{\alpha=1}^n L_\alpha^2$$

is well defined sub-elliptic operator of second order on the frame bundle  $O(M)$ , called the horizontal Laplacian. If  $f \in C^2$  then  $\Delta_{O(M)} f \circ \pi = \Delta f$ . For simplicity, any function  $f$  on  $M$  is lifted to a function  $\tilde{f}$  on  $O(M)$  defined by  $\tilde{f} = f \circ \pi$  which is invariant under the group action by  $O(d)$ .

The following relations will be used in what follows.

$$\tilde{L}_\alpha \tilde{f}(\gamma) = \tilde{L}_\alpha f \circ \pi(\gamma) = e_\alpha^k \frac{\partial f}{\partial x^k}, \quad \text{for } \gamma = (x^i, e_j^k) \in O(M). \quad (4.3)$$

We need the following geometric facts, whose proofs are elementary.

**Lemma 4.3** *For  $\alpha = 1, \dots, n$  we have*

$$\Delta_{O(M)} \tilde{L}_\alpha - \tilde{L}_\alpha \Delta_{O(M)} = \frac{1}{2} \sum_{\beta=1}^n [\tilde{L}_\beta, \tilde{L}_\alpha] \tilde{L}_\beta + \frac{1}{2} \sum_{\beta=1}^n \tilde{L}_\beta [\tilde{L}_\beta, \tilde{L}_\alpha]. \quad (4.4)$$

**Lemma 4.4** *Suppose  $f$  is a smooth function on  $M$  and  $\tilde{f} = f \circ \pi$  is the horizontal lifting of  $f$  to  $O(M)$ .*

1) *For  $\alpha, \beta = 1, \dots, n$*

$$[\tilde{L}_\alpha, \tilde{L}_\beta] \tilde{f} = 0. \quad (4.5)$$

2) We have

$$\sum_{\alpha, \beta=1}^n (\tilde{L}_\alpha \tilde{f})([\tilde{L}_\beta, \tilde{L}_\alpha] \tilde{L}_\beta \tilde{f}) = Ric(\nabla f, \nabla f), \quad (4.6)$$

where  $Ric$  is the Ricci curvature.

3) We also have

$$\Delta_{O(M)} \tilde{L}_\alpha \tilde{f} - \tilde{L}_\alpha \Delta_{O(M)} \tilde{f} = \frac{1}{2} \sum_{\beta=1}^n [\tilde{L}_\beta, \tilde{L}_\alpha] \tilde{L}_\beta \tilde{f}. \quad (4.7)$$

**Proof.** The first identity (4.5) follows from the torsion-free condition. To prove (4.6) we choose a local coordinate which is orthonormal and  $dg_{ij} = 0$  (so that  $\Gamma_{ij}^k = 0$ ) at the point we evaluate tensors, thus

$$\begin{aligned} \tilde{L}_\alpha \tilde{L}_\beta \tilde{L}_\beta \tilde{f} &= e_\beta^j e_\beta^i e_\alpha^q \frac{\partial^3 f}{\partial x^q \partial x^i \partial x^j} - \frac{\partial \Gamma_{ij}^k}{\partial x^q} e_\alpha^q e_\beta^i e_\beta^j \frac{\partial f}{\partial x^k}, \\ \tilde{L}_\beta \tilde{L}_\alpha \tilde{L}_\beta \tilde{f} &= e_\alpha^j e_\beta^i e_\beta^q \frac{\partial^3 f}{\partial x^q \partial x^i \partial x^j} - e_\beta^q e_\alpha^i e_\beta^j \frac{\partial \Gamma_{ij}^k}{\partial x^q} \frac{\partial f}{\partial x^k}, \end{aligned}$$

and therefore

$$[\tilde{L}_\beta, \tilde{L}_\alpha] \tilde{L}_\beta \tilde{f} = \left( \frac{\partial \Gamma_{ij}^k}{\partial x^q} e_\alpha^q e_\beta^i e_\beta^j - e_\alpha^i e_\beta^q e_\beta^j \frac{\partial \Gamma_{ij}^k}{\partial x^q} \right) \frac{\partial f}{\partial x^k},$$

which yields (4.6). (4.7) comes from (4.4) and (4.5). ■

Consider the following stochastic differential equation

$$d\varphi(t) = \sum_{\alpha=1}^n \tilde{L}_\alpha(\varphi(t)) \circ dw_t^\alpha, \quad \varphi(0) = \gamma \in O(M), \quad (4.8)$$

on the classical Wiener space  $(\Omega, \mathcal{F}, \mathbb{P})$  of dimension  $n$ . The stochastic flow associated with (4.8) is denoted by  $\{\varphi(t, \cdot, \gamma) : t \geq 0\}$ , which is a diffusion process in  $O(M)$  with the infinitesimal generator

$$\frac{1}{2} \Delta_{O(M)} = \frac{1}{2} \sum_{\alpha=1}^n \tilde{L}_\alpha \circ \tilde{L}_\alpha,$$

in the sense that

$$M_t^f = f(t, \varphi(t)) - f(0, \varphi(0)) - \int_0^t \frac{1}{2} \Delta_{O(M)} f(s, \varphi(s)) ds$$

is a local martingale for any  $f \in C^{1,2}(\mathbb{R}_+ \times O(M))$ , and

$$M_t^f = \sum_{\alpha=1}^n \int_0^t (L_\alpha f)(s, \varphi(s)) dw_s^\alpha. \quad (4.9)$$

We may express

$$\varphi(t, w, \gamma) = (X(t, w, \gamma), E(t, w, \gamma)),$$

where  $X(t, w, \gamma) = \pi(\varphi(t, w, \gamma))$ , then  $\{X(t, \cdot, \gamma) : t \geq 0\}$  is a diffusion process on  $M$  starting from  $x = \pi(\gamma)$  with infinitesimal generator  $\frac{1}{2} \Delta$ .  $\{X(t, \cdot, \gamma) : t \geq 0\}$  is a Brownian motion on  $M$  starting from  $x = \pi(\gamma)$ .

In a local coordinate system  $(x^k, e_j^i)$ , write

$$\varphi(t, \cdot, \gamma) = (X^k(t, \cdot, \gamma); E_j^i(t, \cdot, \gamma))$$

so that  $E_\alpha(t) = E_\alpha^i(t) \frac{\partial}{\partial x^i}$ . Then the SDE (4.8) may be written as

$$\begin{cases} dX_t^k = \sum_{\alpha=1}^n E_\alpha^k(t) \circ dw_t^\alpha, \\ dE_j^i(t) = - \sum_{\alpha, \beta, k=1}^n \Gamma(X_t)^i_{\beta k} E_j^k(t) E_\alpha^\beta(t) \circ dw_t^\alpha. \end{cases} \quad (4.10)$$

Let  $F(t) = (F(t)_j^i) = E(t)^{-1}$ . Then  $F(t)E(t) = I$  so that

$$dF_j^i(t) = \sum_{\alpha, \beta, l=1}^n \Gamma(X_t)^l_{\beta j} F_l^i(t) E_\alpha^\beta(t) \circ dw_t^\alpha. \quad (4.11)$$

If  $f \in C^{1,2}(\mathbb{R}_+ \times M)$ , then

$$\begin{aligned} f(T, X_T) &= f(t, X_t) + \int_t^T \sum_{\alpha, k=1}^n E_\alpha^k(s) \frac{\partial f}{\partial x^k}(s, X_s) dw_s^\alpha \\ &\quad + \int_t^T \left( \frac{\partial}{\partial s} + \frac{1}{2} \Delta \right) f(s, X_s) ds, \end{aligned} \quad (4.12)$$

so according to (4.3)

$$\begin{aligned} \tilde{f}(T, X_T) &= \tilde{f}(t, X_t) + \int_t^T \sum_{\alpha=1}^n (\tilde{L}_\alpha \tilde{f})(s, (X_s, E(s))) dw_s^\alpha \\ &\quad + \int_t^T \left( \frac{\partial}{\partial s} + \frac{1}{2} \Delta \right) f(s, X_s) ds. \end{aligned} \quad (4.13)$$

#### 4.1 Gradient estimate

Suppose now  $f$  satisfies the non-linear heat equation

$$\left( \frac{1}{2} \Delta - \frac{\partial}{\partial t} \right) f = -\frac{1}{2} |\nabla f|^2. \quad (4.14)$$

Let  $\tilde{f}$  be the horizontal lifting of  $f$  i.e.  $\tilde{f} = f \circ \pi$ , so that  $\tilde{f}$  satisfies the parabolic equation on  $O(M)$ :

$$\left( \frac{1}{2} \Delta_{O(M)} - \frac{\partial}{\partial t} \right) \tilde{f} = -\frac{1}{2} \sum_{\beta=1}^n |\tilde{L}_\beta \tilde{f}|^2. \quad (4.15)$$

Let  $T > 0$ . Let  $Y_t = f(T - t, X_t)$  and

$$Z_t^\alpha = \sum_{k=1}^n E_\alpha^k(t) \frac{\partial f}{\partial x^k}(t, X_t) = (\tilde{L}_\alpha \tilde{f})(t, (X_t, E(t))), \quad (4.16)$$

for  $\alpha = 1, \dots, n$ . Then

$$|\nabla f(T-t, \cdot)|^2(X_t) = \sum_{\alpha=1}^n |Z_t^\alpha|^2, \quad (4.17)$$

therefore, according to (4.12),

$$Y_T = Y_t + \int_t^T Z_t^\alpha dw_s^\alpha - \frac{1}{2} \int_t^T \sum_{\alpha=1}^n |Z_t^\alpha|^2 ds. \quad (4.18)$$

We will consider (4.18) as a backward stochastic differential equation.

Applying Itô's formula to  $\tilde{L}_\alpha \tilde{f}$  and the stochastic flow  $\varphi(t, \cdot, \gamma)$  to obtain

$$\begin{aligned} dZ_t^\alpha &= \sum_{\beta=1}^n \tilde{L}_\beta (\tilde{L}_\alpha \tilde{f})(t, \varphi(t, \cdot, \gamma)) dw_t^\beta \\ &\quad + \left( \frac{1}{2} \Delta_{O(M)} + \frac{\partial}{\partial t} \right) \tilde{L}_\alpha \tilde{f}(t, \varphi(t, \cdot, \gamma)) dt, \end{aligned} \quad (4.19)$$

so

$$\begin{aligned} d|Z|^2 &= 2 \sum_{\alpha=1}^n Z_t^\alpha dZ_t^\alpha + \sum_{\alpha, \beta=1}^n |\tilde{L}_\beta \tilde{L}_\alpha \tilde{f}|^2(t, \varphi(t, \cdot, \gamma)) dt \\ &= 2 \sum_{\alpha, \beta=1}^n Z_t^\alpha (\tilde{L}_\beta \tilde{L}_\alpha \tilde{f}) dw_t^\beta + \sum_{\alpha, \beta=1}^n |\tilde{L}_\beta \tilde{L}_\alpha \tilde{f}|^2 dt \\ &\quad + 2 \sum_{\alpha=1}^n Z_t^\alpha \left( \frac{1}{2} \Delta_{O(M)} + \frac{\partial}{\partial t} \right) \tilde{L}_\alpha \tilde{f} dt. \end{aligned} \quad (4.20)$$

However, by Lemma 4.3,

$$\begin{aligned} \left( \frac{1}{2} \Delta_{O(M)} + \frac{\partial}{\partial t} \right) \tilde{L}_\alpha \tilde{f} &= \tilde{L}_\alpha \left( \frac{1}{2} \Delta_{O(M)} + \frac{\partial}{\partial t} \right) \tilde{f} + \frac{1}{4} \sum_{\beta=1}^n [\tilde{L}_\beta, \tilde{L}_\alpha] \tilde{L}_\beta \tilde{f} \\ &= - \sum_{\beta=1}^n (\tilde{L}_\beta \tilde{f})(\tilde{L}_\alpha \tilde{L}_\beta \tilde{f}) + \frac{1}{4} \sum_{\beta=1}^n [\tilde{L}_\beta, \tilde{L}_\alpha] \tilde{L}_\beta \tilde{f}, \end{aligned}$$

we therefore have

$$\begin{aligned} d|Z|^2 &= 2 \sum_{\alpha=1}^n Z_t^\alpha \sum_{\beta=1}^n (\tilde{L}_\beta \tilde{L}_\alpha \tilde{f}) (dw_t^\beta - Z_t^\beta dt) \\ &\quad + \sum_{\alpha, \beta=1}^n |\tilde{L}_\beta \tilde{L}_\alpha \tilde{f}|^2 dt + \frac{1}{2} \sum_{\alpha, \beta=1}^n (\tilde{L}_\alpha \tilde{f})([\tilde{L}_\beta, \tilde{L}_\alpha] \tilde{L}_\beta \tilde{f}) dt. \end{aligned}$$

By using Lemma 4.3 we obtain

$$\begin{aligned} d|Z|^2 &= 2 \sum_{\alpha=1}^n Z_t^\alpha \sum_{\beta=1}^n (\tilde{L}_\beta \tilde{L}_\alpha \tilde{f}) (dw_t^\beta - Z_t^\beta dt) \\ &\quad + \sum_{\alpha, \beta=1}^n |\tilde{L}_\beta \tilde{L}_\alpha \tilde{f}|^2 dt + \frac{1}{2} \text{Ric}(\nabla f, \nabla f)(T-t, X_t) dt. \end{aligned} \quad (4.21)$$

Define a probability  $\mathbb{Q}$  by  $\frac{d\mathbb{Q}}{d\mathbb{P}}\Big|_{\mathcal{F}_T} = R_T$  where

$$R_t = \exp \left[ \int_0^t Z^\beta dw^\beta - \frac{1}{2} \int_0^t |Z|^2 ds \right].$$

Then

$$Y_T = Y_t + \int_t^T Z_t^\alpha d\tilde{w}_s^\alpha + \frac{1}{2} \int_t^T \sum_{\alpha=1}^n |Z_t^\alpha|^2 ds,$$

hence

$$\mathbb{E}^{\mathbb{Q}} \left\{ \int_t^T |Z_s|^2 ds \middle| \mathcal{F}_t \right\} \leq 4 \|f_0\|_\infty. \quad (4.22)$$

But on the other hand  $e^{\frac{Kt}{2}} |Z_t|^2$  is submartingale under  $\mathbb{Q}$ , thus

$$\begin{aligned} \mathbb{E}^{\mathbb{Q}} \left\{ \int_t^T |Z_s|^2 ds \middle| \mathcal{F}_t \right\} &= \int_t^T \mathbb{E}^{\mathbb{Q}} \{ |Z_s|^2 \middle| \mathcal{F}_t \} ds \\ &\geq e^{\frac{Kt}{2}} |Z_t|^2 \int_t^T e^{-\frac{Ks}{2}} ds \\ &= \frac{1 - e^{-\frac{K}{2}(T-t)}}{\frac{K}{2}} |Z_t|^2, \end{aligned}$$

which yields that

$$|Z_t|^2 \leq \frac{2K}{1 - e^{-\frac{K}{2}(T-t)}} \|f_0\|_\infty,$$

and hence (4.2).

## 5 Li-Yau's estimate

In this section we prove Theorem 1.4. Thus,  $u$  is a positive solution to the heat equation

$$\left( \frac{1}{2} \Delta - \frac{\partial}{\partial t} \right) u = 0, \quad \text{on } [0, \infty) \times M, \quad (5.1)$$

where  $M$  is a complete Riemannian manifold of dimension  $n$ , with non-negative Ricci curvature. Then  $f = \log u$  is a solution to the semi-linear heat equation

$$\left( \frac{1}{2} \Delta - \frac{\partial}{\partial t} \right) f = -\frac{1}{2} |\nabla f|^2, \quad f(0, \cdot) = f_0. \quad (5.2)$$

Taking derivative in the parabolic equation (5.2) with respect to the time parameter  $t$  one obtains

$$\frac{\partial}{\partial t} f_t = L f_t, \quad (5.3)$$

where

$$L = \frac{1}{2} \Delta + \nabla f \cdot \nabla.$$

By using the Bochner identity one can verify that

$$\frac{\partial}{\partial t} |\nabla f|^2 = L |\nabla f|^2 - |\nabla \nabla f|^2 - 2\text{Ric}(\nabla f, \nabla f) . \quad (5.4)$$

Since  $\Delta f$  is the trace of the Hessian  $\nabla \nabla f$  so that  $|\nabla \nabla f|^2 \geq \frac{1}{n} (\Delta f)^2$ , thus, since the Ricci curvature is non-negative, then

$$\frac{\partial}{\partial t} |\nabla f|^2 \leq L |\nabla f|^2 - \frac{1}{n} (\Delta f)^2 . \quad (5.5)$$

Let

$$G = -\Delta f = |\nabla f|^2 - 2f_t .$$

By combining (5.3) and (5.5) together, we obtain

$$\frac{\partial}{\partial t} G \leq LG - \frac{1}{n} G^2 . \quad (5.6)$$

Suppose that  $C > 0$  and  $-\nabla \log u_0 \leq C$ . Set

$$F = \left( \frac{t}{n} + \frac{1}{C} \right) (-\Delta f) .$$

Since

$$\begin{aligned} \left( \frac{\partial}{\partial t} - L \right) F &= \frac{1}{n} G + \left( \frac{t}{n} + \frac{1}{C} \right) \left( \frac{\partial}{\partial t} - L \right) G \\ &\leq \frac{1}{n} G - \left( \frac{t}{n} + \frac{1}{C} \right) \frac{1}{n} G^2 \\ &= \frac{1}{n} G (1 - F) , \end{aligned}$$

and therefore

$$\left( L - \frac{\partial}{\partial t} \right) (F - 1) \geq \frac{1}{n} G (F - 1) .$$

As  $-\Delta \log u_0 \leq C$ ,  $(F - 1)(0, \cdot) \leq 0$ . Applying the maximum principle,  $F - 1 \leq 0$ , from which we obtain the estimate in Theorem 1.4.

**Corollary 5.1** *Suppose  $u$  is a positive solution to (5.1), then the following Harnack inequality holds:*

$$\frac{u(t, x)}{u(t + s, y)} \leq \exp \left[ \int_t^{t+s} K(\sigma, \frac{\rho}{s}) d\sigma \right]$$

where

$$K(t, \alpha) = \sup_{Y: \psi(t, Y) \geq 0} \left\{ \alpha \sqrt{\psi(t, Y)} - Y \right\}$$

and

$$\psi(t, Y) = 2Y + \frac{C}{\frac{t}{n}C + 1} .$$

Thus

$$\frac{u(t, x)}{u(t + s, y)} \leq \left( \frac{\frac{1}{C} + \frac{1}{n}(t + s)}{\frac{1}{C} + \frac{1}{n}t} \right)^{\frac{n}{2}} \exp \left[ \frac{r(x, y)^2}{2s} \right] .$$

This follows by integrating the gradient estimates in Theorem 1.4 along geodesics, see [2] for details.

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